CLAIMS

We claim:

1. A method for analyzing multivariate images, comprising:

a) providing a data matrix **D** containing measured spectral data,

b) transforming the data matrix **D**, using a wavelet transform, to obtain a transformed data matrix $\tilde{\mathbf{D}}$,

c) performing an image analysis on the transformed data matrix $\tilde{\mathbf{D}}$ to obtain a transformed concentration matrix $\tilde{\mathbf{C}}$ and a spectral shapes matrix **S**, and

d) computing a concentration matrix **C** from the transformed concentration matrix $\tilde{\mathbf{C}}$.

2. The method of Claim 1, wherein the data matrix **D** comprises a total of *j* blocks of data $\mathbf{D}_i$, each data block $\mathbf{D}_i$ thereby providing a concentration block $\mathbf{C}_i$ in step a), and wherein steps a) through d) are repeated sequentially until the concentration matrix **C** is accumulated blockwise, according to

$$\mathbf{C} = \begin{bmatrix} \mathbf{C}_1 & \mathbf{C}_2 & \cdots & \mathbf{C}_{j-1} & \mathbf{C}_j \end{bmatrix}.$$

3. The method of Claim 1, wherein the wavelet transform comprises a Haar transform.

4. The method of Claim 1, further comprising thresholding the wavelet coefficients of the transformed data matrix $\tilde{\mathbf{D}}$.

5. The method of Claim 4, wherein the thresholding comprises decimating the detail coefficients.

6. The method of Claim 1, wherein the image analysis of step c) comprises an alternating least squares analysis and the transformed concentration matrix $\tilde{\mathbf{C}}$ and the spectral shapes matrix **S** are obtained from a constrained least squares solution of $\min_{\tilde{\mathbf{C}},\mathbf{S}} \left\| \tilde{\mathbf{D}} - \tilde{\mathbf{C}}\mathbf{S}^{\mathrm{T}} \right\|_{\mathrm{F}}$.

7. The method of Claim 6, wherein the alternating least squares analysis comprises a transformed non-negativity constraint.

8. The method of Claim 1, wherein the computing step d) comprises applying an inverse wavelet transform to the transformed concentration matrix $\tilde{\mathbf{C}}$ to provide the concentration matrix **C**.

9. The method of Claim 1, wherein the computing step d) comprises projecting the data matrix **D** from step a) onto the spectral shapes matrix **S** from step c), according to $\min_{\mathbf{C}}\left\|\mathbf{D}-\mathbf{C}\mathbf{S}^{\mathrm{T}}\right\|_{F}$.

10. A method for analyzing multivariate images, comprising:

a) providing a data factor matrix **A** and a data factor matrix **B** obtained from a factorization of measured spectral data **D**,

b) transforming the data factor matrix **A**, using a wavelet transform, to obtain a transformed data factor matrix $\tilde{\mathbf{A}}$,

c) performing an image analysis on the transformed data factor matrix $\tilde{\mathbf{A}}$ and data factor matrix **B** to obtain a transformed concentration matrix $\tilde{\mathbf{C}}$ and a spectral shapes matrix **S**, and

d) computing a concentration matrix **C** from the transformed concentration matrix $\tilde{\mathbf{C}}$.

11. The method of Claim 10, wherein the data factor matrix **A** comprises a total of j blocks of data factors $\mathbf{A}_i$ and the data factor matrix **B** comprises k blocks of data factors $\mathbf{B}_i$, thereby providing a concentration block $\mathbf{C}_i$ in step d), and wherein steps a) through d) are repeated sequentially until the concentration matrix **C** is accumulated blockwise, according to $\mathbf{C}=\left[\mathbf{C}_1 \quad \mathbf{C}_2 \quad \cdots \quad \mathbf{C}_{j-1} \quad \mathbf{C}_j\right]$.

12. The method of Claim 10, wherein the wavelet transform comprises a Haar transform.

13. The method of Claim 10, further comprising thresholding the wavelet coefficients of the transformed data factor matrix $\tilde{\mathbf{A}}$.

14. The method of Claim 13, wherein the thresholding comprises decimating the detail coefficients.

15. The method of Claim 10, wherein the image analysis of step c) comprises an alternating least squares analysis and the transformed concentration matrix $\tilde{\mathbf{C}}$ and the spectral shapes matrix **S** are obtained from a constrained least squares solution of $\min_{\tilde{\mathbf{C}},\mathbf{S}} \left\| \tilde{\mathbf{A}}\mathbf{B}^T - \tilde{\mathbf{C}}\mathbf{S}^T \right\|_F$.

16. The method of Claim 15, wherein the alternating least squares analysis comprises a transformed non-negativity constraint.

17. The method of Claim 10, wherein the computing step d) comprises applying an inverse wavelet transform to the transformed concentration matrix $\tilde{\mathbf{C}}$ to provide the concentration matrix **C**.

18. The method of Claim 10, wherein the computing step d) comprises projecting the product of the data factor matrix **A** and the data factor matrix **B** from step a) onto the spectral shapes matrix **S** from step c), according to $\min_{\mathbf{C}} \left\| \mathbf{A}\mathbf{B}^T - \mathbf{C}\mathbf{S}^T \right\|_F$ and subject to appropriate constraints.

19. The method of Claim 10, wherein the data factor matrix **A** comprises a scores matrix **T** and the data factor matrix **B** comprises a loadings matrix **P**, and wherein **T** and **P** are obtained from a principal components analysis of the measured spectral data **D**, according to $\mathbf{D} = \mathbf{T}\mathbf{P}^T$.

20. The method of Claim 19, wherein **T** and **P** represent the significant components of the principal components.